

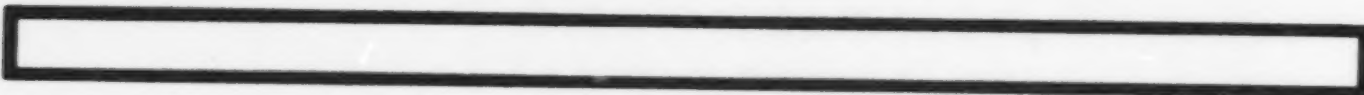
Rocky Mountain Acid Deposition Modeling
Assessment Project--Goals and Current Status

Systems Applications, Inc., San Rafael, CA

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THE ROCKY MOUNTAIN ACID DEPOSITION
MODELING ASSESSMENT PROJECT--
GOALS AND CURRENT STATUS

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The objective of the Rocky Mountain Acid Deposition Modeling Assessment Project is to assemble an acid deposition model based on currently available air quality and meteorological models and modules that adequately describe the processes of acid deposition in the Rocky Mountain region. The model would be used in-house by Federal and State agencies in the western states. After reviewing and selecting mesoscale meteorological and acid deposition models appropriate to application in the Rocky Mountain region, three alternative modeling approaches were identified. The modeling approach taken will depend upon the recommendations of the regulatory agencies. The resulting modeling system should be operational by the end of summer 1987.

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1 INTRODUCTION

Acid deposition has recently become an increasing concern in the western United States (World Resources Institute, 1985). Although this problem may not be as acute in the West as it is in the East, it has nevertheless become a concern of regulatory agencies because of the high sensitivity of western lakes at high altitudes and the rapid industrial growth expected to occur in certain areas of the West. An example of such an area is the region known as the Overthrust Belt in southwestern Wyoming. Several planned energy-related projects, including natural gas sweetening plants and coal-fired power plants, may considerably increase the emission of acid precursors in northeastern Utah and northwestern Colorado and significantly affect ecosystems in the sensitive Rocky Mountain areas.

Under the 1977 Clean Air Act, the U.S. Environmental Protection Agency (EPA), along with other federal and state agencies, is required to preserve and protect air quality throughout the country. As part of the Prevention of Significant Deterioration (PSD) permitting processes, federal and state agencies are required to evaluate potential impacts of new emission sources. In particular, Section 165 of the Clean Air Act stipulates that, except in specially regulated instances, PSD increments shall not be exceeded and air quality-related values (AQRVs) shall not be adversely affected. Air-quality-related concerns range from near-source plume blight to regional-scale acid deposition problems. By law, the Federal Land Manager of Class I areas has a responsibility to protect air-quality-related values within those areas. New source permits cannot be issued by the EPA or the states when the Federal Manager concludes that adverse impacts on air quality or air-quality-related values will occur. The locations of the 92 Class I areas in the western states are shown in Figure 1 while Table 1 identifies these areas.

Study Objectives

The objective of the Rocky Mountain Acid Deposition Modeling Assessment Project is to assemble an acid deposition model based on currently available air quality and meteorological models and modules that adequately describe the processes of acid deposition in the Rocky Mountain region. The model would be used by federal and state agencies in the western states. This effort differs from other acid deposition model development efforts, such as the NCAR/RADM, in that the model is to be designed

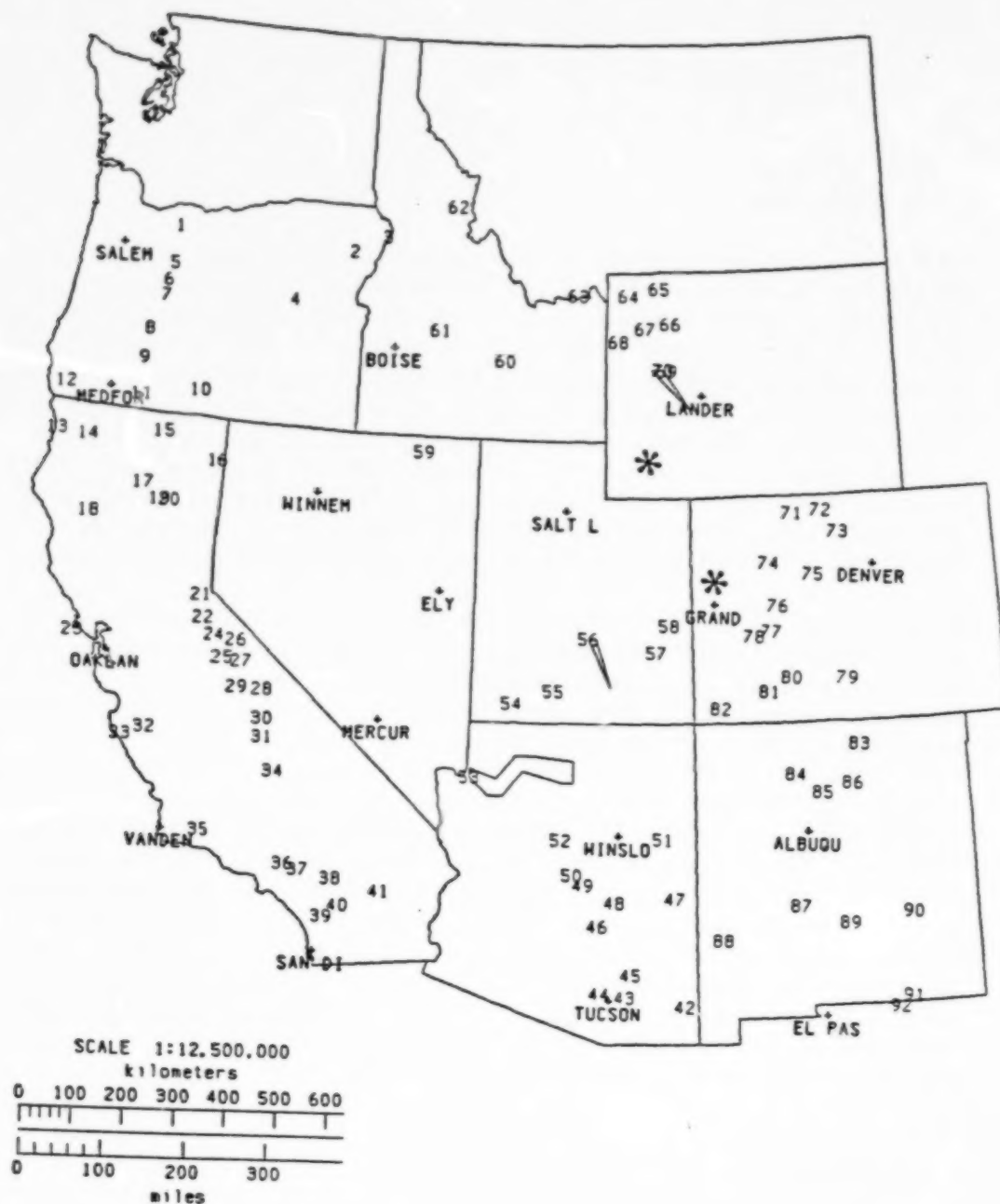


FIGURE 1. Class I areas and upper-air meteorological stations located in the West, exclusive of Washington and Montana. The locations of the first two application scenarios (in Wyoming and Colorado) are indicated by large asterisks. (Key to locations is in Table 1.)

TABLE 1. Key to Class I Areas located in the West.

NO	NAME
1	Mount Hood Wilderness
2	Eagle Cap Wilderness
3	Bells Canyon Wilderness
4	Strawberry Mountain Wilderness
5	Mt. Jefferson Wilderness
6	Mt. Washington Wilderness
7	Three Sisters Wilderness
8	Diamond Peak Wilderness
9	Crater Lake National Park
10	Gearhart Mountain Wilderness
11	Mountain Lakes Wilderness
12	Kalmiopsis Wilderness
13	Redwood National Park
14	Marble Mountain Wilderness
15	Lava Beds Wilderness
16	South Warner Wilderness
17	Thousand Lakes Wilderness
18	Yolla-Bolly - Middle Eel Wilderness
19	Lassen Volcanic National Park
20	Caribou Wilderness
21	Desolation Wilderness
22	Mokelumme Wilderness
23	Point Reyes Wilderness
24	Emigrant Wilderness
25	Yosemite National Park
26	Hoover Wilderness
27	Minarets Wilderness
28	John Muir Wilderness
29	Kaiser Wilderness
30	Kings Canyon National Park
31	Sequoia National Park
32	Pinnacles Wilderness
33	Ventana Wilderness
34	Dome Land Wilderness
35	San Rafael Wilderness
36	San Gabriel Wilderness
37	Cucamonga Wilderness
38	San Geronio Wilderness
39	Agua Tibia Wilderness
40	San Jacinto Wilderness
41	Joshua Tree Wilderness
42	Chiricahua Wilderness
43	Saguaro Wilderness - East
44	Saguaro Wilderness - West
45	Galiuro Wilderness
46	Superstition Wilderness
47	Mt. Baldy Wilderness
48	Sierra Ancha Wilderness
49	Mazatzal Wilderness
50	Pine Mountain Wilderness

TABLE 1. Concluded.

NO	NAME
51	Petrified Forest National Park
52	Sycamore Canyon Wilderness
53	Grand Canyon National Park
54	Zion National Park
55	Bryce Canyon National Park
56	Capitol Reef National Park
57	Canyonlands National Park
58	Arches National Park
59	Jarbridge Wilderness
60	Craters of the Moon Wilderness
61	Sawtooth Wilderness
62	Selway Bitterroot Wilderness
63	Red Rock Lakes Wilderness
64	Yellowstone National Park
65	North Absaroka Wilderness
66	Washakie Wilderness
67	Teton Wilderness
68	Grand Teton National Park
69	Fitzpatrick Wilderness
70	Bridger Wilderness
71	Mount Zirkel Wilderness
72	Rawah Wilderness
73	Rocky Mountain National Park
74	Flat Tops Wilderness
75	Eagles Nest Wilderness
76	Maroon-Bells Snowmass Wilderness
77	West Elk Wilderness
78	Black Canyon of the Gunnison Wilder.
79	Great Sand Dunes Wilderness
80	La Garita Wilderness
81	Weminuche Wilderness
82	Mesa Verde National Park
83	Wheeler Peak Wilderness
84	San Pedro Parks Wilderness
85	Bandelier Wilderness
86	Pecos Wilderness
87	Bosque del Apache Wilderness
88	Gila Wilderness
89	White Mountain Wilderness
90	Salt Creek Wilderness
91	Carlsbad Caverns National Parks
92	Guadalupe National Park

specifically for use and application by western regulatory agencies to estimate acid deposition impacts from proposed new sources. The Western Acid Deposition Task Force provided the following guidelines on the design of the model.

The anticipated use of this model is to analyze permit applications and evaluate urban development plans. The model is thus expected to simulate impacts of various air pollutants from both point and area sources.

A typical modeling area will cover approximately 200 km to 300 km on the side to have the ability to calculate impacts from new sources within relatively short distances of Class I areas.

The model should be able to handle events over long time periods, such as calculating seasonal and/or annual averages, in order to obtain cumulative impacts from both chronic and episodic events.

The model should be able to simulate transport, diffusion, transformation, and deposition of pollutants over complex terrain in the Rocky Mountain region with relatively sparse NWS upper-air soundings.

The model should be able to predict acid deposition fluxes of sulfur and nitrogen species.

Treatment of both gas- and aqueous-phase chemistry is desirable.

The model should treat orographic effects on precipitation, including enhanced precipitation rates, snowfall, and ice-phase processes.

The modeling system should be simple enough to be used by a regulatory agency on a mid-sized minicomputer.

Study Organization

The Rocky Mountain Acid Deposition Modeling Assessment Project is divided into three main tasks and three optional tasks as follows.

Task 1

Review and selection of candidate mesoscale meteorological models

Review and selection of candidate acid deposition models

Selection of first application scenarios

Task 2

Aquisition, testing, and evaluation of model components

Assembly of hybrid modeling system

Task 3

Delivery and installation of modeling system on the EPA's computer

Optional Task 1

Assembly of an aerometric data base suitable for model operation and evaluation

Optional Task 2

Detailed evaluation studies of the modeling system

Optional Task 3

Refinement and adaptation of the modeling system

At this time (August 1986) task 1 has been completed. The following draft documents were completed under this task: (1) a review of mesoscale meteorological models that can calculate wind fields in complex terrain (Morris et al., 1986a), (2) a review of acid deposition models that could serve as the basis for a Rocky Mountain Model (Morris et al., 1986b), and (3) a description of some typical application scenarios in the Rocky Mountain west (Morris, 1986). These draft documents also recommend models that would be most suitable for the development of a model for Rocky Mountain acid deposition issues. These three documents have been combined to form a final report entitled "Rocky Mountain Acid Deposition Modeling Assessment, Review of Existing Mesoscale Models for Use in Complex Terrain" (Morris and Kessler, 1987), available through NTIS.

At meetings in Colorado on 28 and 29 July 1986, Systems Applications' staff met with EPA staff and several members of the Western Atmospheric Deposition Task Force (WADTF) and its Atmospheric Processes Work Group (WADTF/AP) to review progress on the project and to collect comments before proceeding with the selection of meteorological and acid deposition models for testing (task 2) and implementation and documentation (task 3). Several issues were identified at that meeting that may help to focus

the conceptual design of the modeling system. Before embarking on task 2 of the project, written comments on the conceptual design of the model were requested from the regulatory agencies for whom the model is designed.

2 TYPES OF APPLICATIONS FOR THE PROPOSED MODEL

The primary purpose of the Rocky Mountain Acid Deposition Model is to determine whether acid deposition from new sources and urban growth will adversely affect ecological systems in sensitive areas within complex terrain in the Rocky Mountains. To determine this, the model must predict the total cumulative deposition of sulfates and nitrates, as well as the contribution of the new source. Acid deposition modeling in the Rocky Mountains is further complicated by the complex terrain in the region, and the fact that many of the sensitive lakes are located at higher elevations, where orographic effects on precipitation increase wet deposition of pollutants.

The two application scenarios described here represent the types of new sources that have been proposed in the western Rockies. They include sufficiently diverse sources and emission characteristics to test the model's ability to predict cumulative and source-specific acid deposition at the sensitive areas.

One scenario includes a shale oil plant in western Colorado, the other includes three gas treatment plants in southwestern Wyoming. The relationship between the locations of these sources and the PSD class I areas and acid-sensitive areas in the West is shown in Figures 1 and 2.

Application Scenario No. 1--Colorado Shale Oil Plant

The first application scenario is the Chevron Clear Creek Shale Oil Project (CCSOP), located in the south-central portion of the Piceance Basin in Garfield County, Colorado. This site is approximately 40 miles north-east of Grand Junction and 26 miles north of DeBeque. The closest PSD class I area is the Flat Tops Wilderness Area, which lies approximately 50 to 55 miles to the northeast of the CCOSP site. Figure 2 shows the relationship between the CCSOP and class I areas within a rather large (750 km x 750 km) region.

For this application scenario the Flat Tops and Maroon-Belles Wilderness Areas will be the primary receptors of interest; however, estimates of cumulative and source-specific acid deposition would be calculated at all PSD class I and sensitive areas.

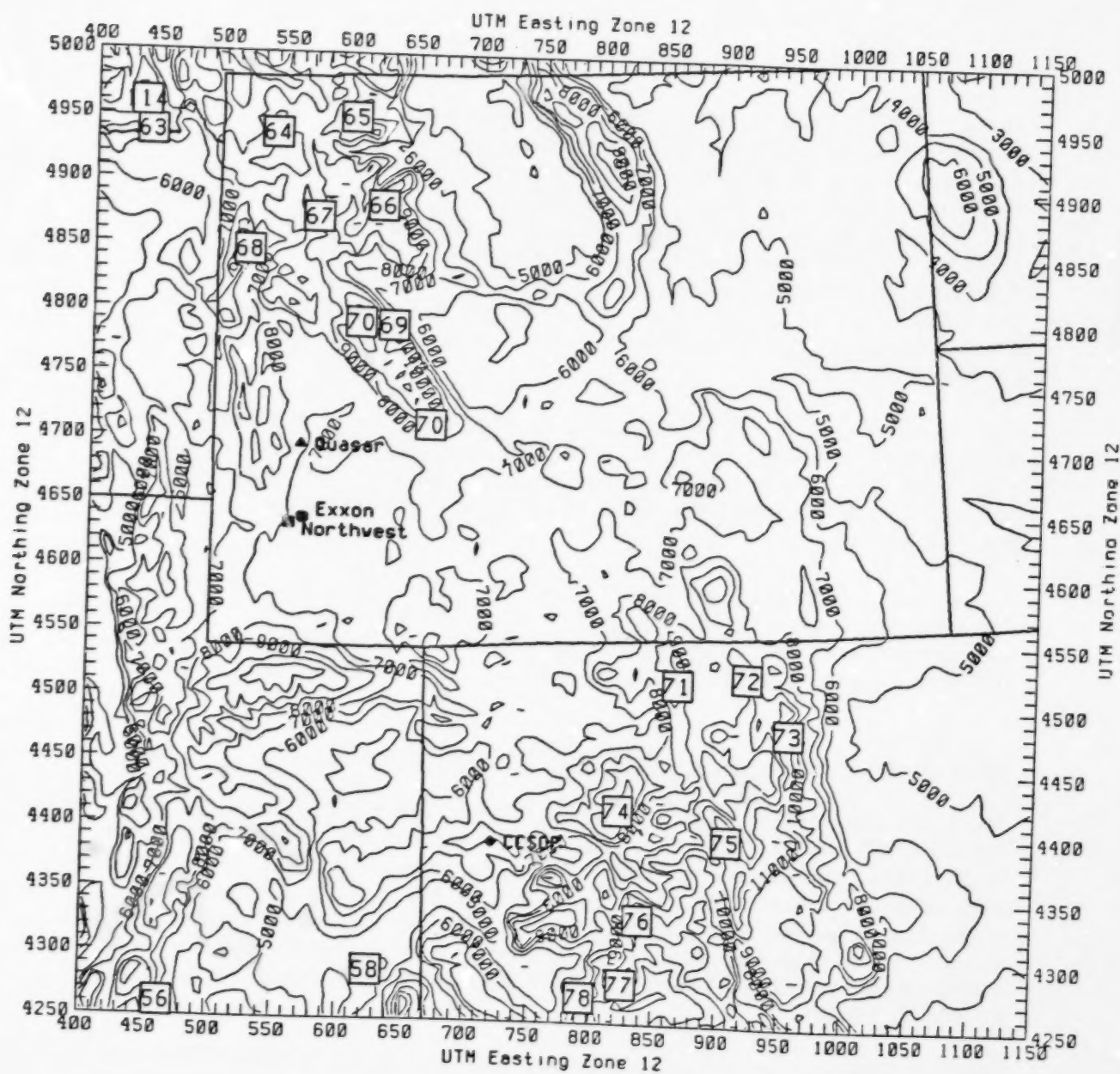


FIGURE 2. Relationship between application scenarios and PSD class I areas (see Table 1 for key). Terrain elevations are in feet above mean sea level.

The Flat Tops Wilderness Area includes several lakes that are susceptible to adverse effects from acid deposition because of low alkalinity (Turk and Adams, 1982). This area is one of the first major orographic barriers to air masses resulting from the predominantly southwest winds over the Piceance Basin. Thus, emissions from the CCSOP may be carried up to the Flat Tops Wilderness Area and precipitated out before they have been effectively dispersed.

Figures 3 and 4 show the terrain in a mesoscale region (250 km x 250 km) containing the CCSOP site and the Flat Tops and Maroon-Belles Wilderness Area. This region is dominated by a series of ridges and valleys leading up to the Flat Tops Wilderness Area. Correct specification of the three-dimensional wind field and spatial variability of precipitation will be an important factor in modeling this scenario.

The extraction of oil from oil shale through combustion results mostly in emissions of NO_x and CO . This application scenario will illustrate the model's ability to predict nitrogen deposition at source-receptor distances of about 80 km. Because of the low solubility of NO and NO_2 , wet deposition of nitrogen is usually in the form of nitrates or nitric acids. Thus it will be important to characterize the conversion of the emitted NO_x to nitrates. The gas-phase conversion of NO_x to nitrates is relatively rapid and depends on the availability of oxidizing precursors in the atmosphere. Nitrate formation in precipitation depends on a combination of gas-phase, gas-particle, and aqueous-phase reactions, with both reversible and irreversible conversions. Thus the correct specification of the background reactivity and precipitation patterns will be important for this application scenario.

Application Scenario No. 2--Wyoming Gas Treatment Plants

The second application scenario includes three gas treatment plants located in the Riley Ridge area of southwestern Wyoming. These plants are the Exxon Shute Creek plant approximately five miles north of Opal, the Northwest/Mobil Craven Creek plant approximately 12 miles north-northeast of Opal, and the Quasar East Dry Basin plant approximately nine miles southwest of Big Piney. The closest PSD class I areas are the Bridger and Fitzpatrick wilderness areas located in the Wind River Range (Figure 2). These wilderness areas are approximately 50 miles northeast of the Quasar East Dry Basin plant site, and approximately 80-85 miles north-northeast from the Exxon and Northwest/Mobil plant sites. Other nearby class I areas include Grand Teton National Park and the Teton Wilderness Area, located due north from the plant sites (Figure 2).

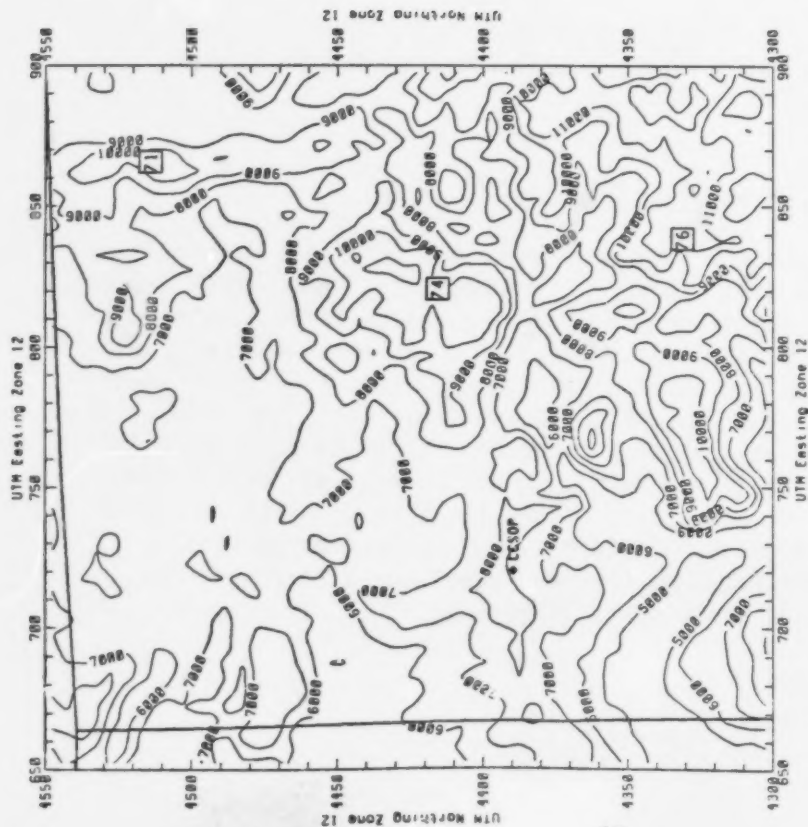


FIGURE 3. Application scenario #1 mesoscale region containing the Clear Creek shale oil plant (CCSOP) and two PSD class I areas--Flat Tops (74) and Maroon-Bells Snowmass Wilderness (76).

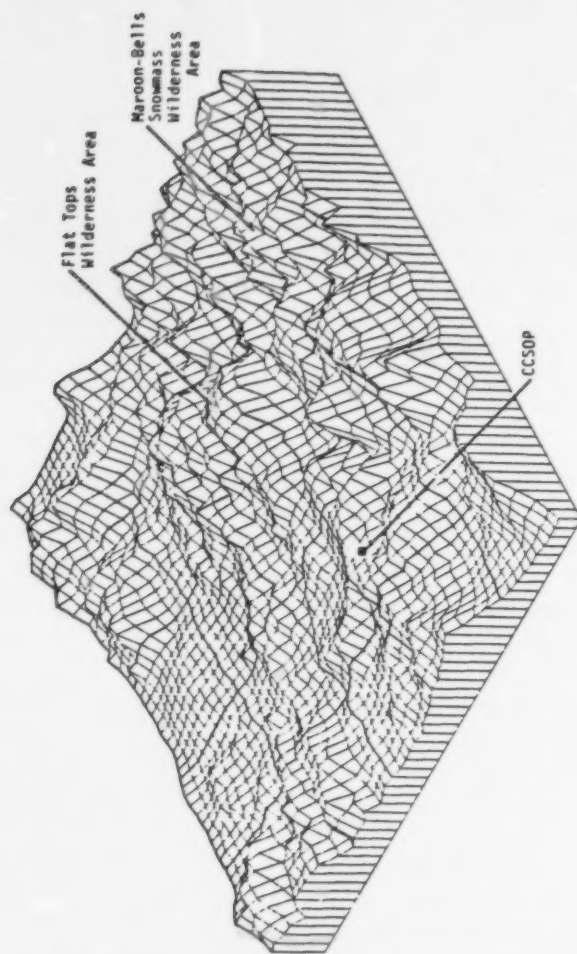


FIGURE 4. Three-dimensional perspective of terrain showing the first application scenario source and class I receptor areas.

Figures 5 and 6 show the terrain in a mesoscale region (250 km by 250 km) containing the gas plant sites and the Bridger and Fitzpatrick wilderness areas. The pollutants would be carried across a relatively flat area by southwest winds until they encounter the Wind River Range, where the air parcel would be forced upward, possibly resulting in orographic precipitation when the saturation level is achieved.

The main pollutant emitted from these sources is sulfur dioxide; some nitrogen oxides are also emitted. This scenario differs from the first because of the proximity of several major sources, including the Naughton and Jim Bridger power plants, the Opal gas plant, and other gas and chemical plants.

The gas-phase oxidation of SO_2 to sulfates is rather slow. However in the presence of hydrogen peroxide and other oxidizing agents, the aqueous-phase oxidation of SO_2 to sulfates is almost instantaneous. Thus, for this application scenario the transformation of the emitted SO_2 to sulfate will most likely be limited to the amount of hydrogen peroxide and other oxidizers available. It will be crucial to obtain an estimate of the oxidizing precursors and cloud amounts in order to properly estimate the proper SO_2 oxidation rate and resultant sulfate deposition.

3 REVIEW AND SELECTION OF APPROPRIATE MESOSCALE METEOROLOGICAL MODELS

Over 60 mesoscale meteorological models were reviewed to select the most appropriate candidates for application to the Rocky Mountain region (Morris et al., 1986a). This initial selection was based on a few critical factors: (1) the ability of the model to simulate mesoscale meteorological processes over complex terrain; (2) flexibility and adaptability of the model, and (3) computational requirements.

These minimal requirements eliminated all but seven diagnostic (mass consistent) wind models and six prognostic (primitive equation) meteorological models. Table 2 shows the relative ranking of the diagnostic models and prognostic models as a result of the technical merit analysis.

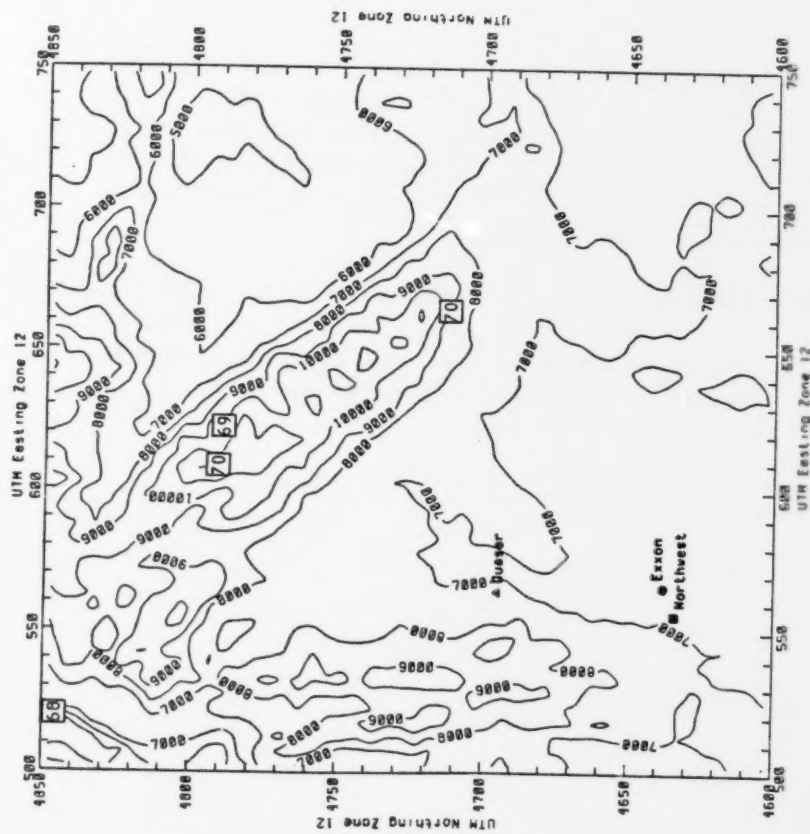


FIGURE 5. Application scenario #2 mesoscale region containing the three gas treatment plants and two PSD class I areas--Bridger Wilderness Area (area between the two boxes with number 70) and Fitzpatrick Wilderness Area (69), both in the Wind River Mountains.

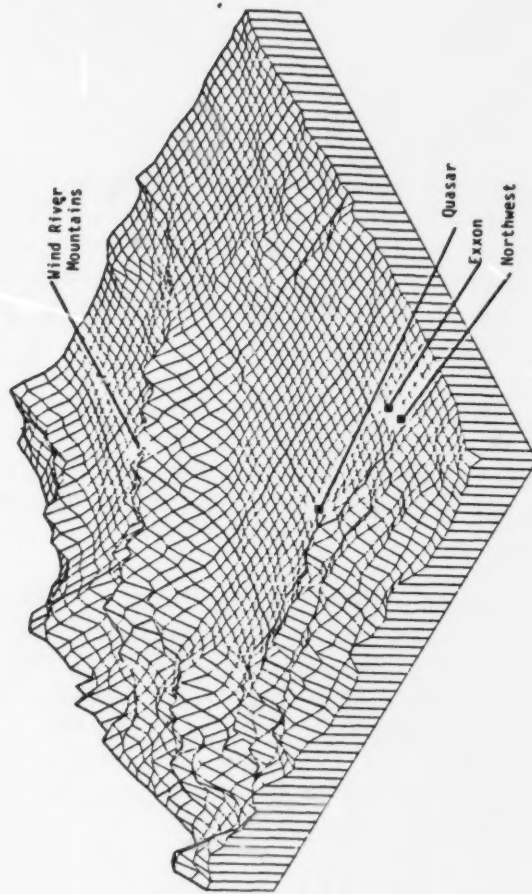


FIGURE 6. Three-dimensional perspective of terrain showing the sources in the second application scenario and the Wind River Mountains, which include the class I receptor areas.

TABLE 2. Relative ranking of diagnostic and prognostic mesoscale meteorological models.

<u>Diagnostic Models</u>	<u>Prognostic Models</u>
PNL/MELSAR-MET	NCAR/MM4
SAI/CTWM	MESO/MASS
SAI/MVWM	CSU/MESOSCALE
LANL/ATMOS1	NOAA/ERL
LLNL/MATHEW	LANL/HOTMAC
CIT/WIND	DREXEL/NCAR
SRI/DIAGNOSTIC	

4 REVIEW AND SELECTION OF AN APPROPRIATE ACID DEPOSITION MODEL

Regional and mesoscale acid deposition models were surveyed and reviewed for potential candidates to apply to the Rocky Mountain Region (Morris et al., 1986b). The regional and mesoscale acid deposition models that have been developed in the past decade can be divided into four categories according to model framework: fixed-coordinate Eulerian models, moving-coordinate Lagrangian models, hybrid models that merge aspects of both the Lagrangian and Eulerian concepts, and statistical models that are used primarily for long-term averages. Because of the complex terrain in the Rocky Mountains and the importance of nonlinear chemical and deposition processes in acid deposition, the use of a statistical model may not be appropriate for this application.

The technical merits of the models under review were compared by assigning a relative score to the key components of each model (transport, dispersion, chemical transformation, wet- and dry-deposition). Based on this analysis, the Eulerian and Lagrangian acid deposition models were ranked as shown in Table 3.

TABLE 3. Relative ranking of Eulerian and Lagrangian acid deposition models.

<u>Eulerian/Hybrid Models</u>	<u>Lagrangian Models</u>
NCAR/RADM	SAI/CCADM
ERT/ADOM	ERT/MESOPUFF-II
UK/STEM-II	SAI/RIVAD
EPA/ROM	PNL/MELSAR-POLUT
SAI/RTM-III	
SAI/RTM-II	
UK/STEM	

5 PROPOSED MODELING APPROACHES

The conceptual design for the Rocky Mountain Acid Deposition Model envisions a hybrid modeling system consisting of a meteorological model as a driver for an acid deposition model. Models will be developed to handle both mesoscale and regional issues.

Since cost considerations preclude the use of dynamic wind field models, we have recommended using the Limited-Area Fine-Mesh (LFM) of the National Meteorological Center, the data for which are archived by the National Center for Atmospheric Research in Boulder, to characterize regional-scale wind fields, and a diagnostic (mass-conserving) wind model to characterize winds within a mesoscale modeling region. The LFM wind data is rather coarse (127 km) and can only characterize the regional upper level flow in the Rocky Mountains, while the diagnostic model will handle the complicated flows within the complex-terrain mesoscale region.

The wind fields will determine where pollutants are transported, while the acid deposition model will calculate the processes of dispersion, chemical transformation, dry deposition and wet deposition. Two types of acid deposition models have been recommended: a Lagrangian (plume segment or puff) and an Eulerian (grid) model. We have proposed three conceptual designs, from which the regulatory agencies will have an opportunity to choose their preferred approach. The three proposed modeling approaches differ in whether Lagrangian or Eulerian models are used for both regional and mesoscale modeling. Several aspects of the approaches are compared in Table 4.

TABLE 4. Comparison of the attributes of the three alternatives for the Rocky Mountain Acid Deposition Model.

Attribute	Alternative 1: Fully Lagrangian	Alternative 2: Lagrangian/Eulerian	Alternative 3: Nested Eulerian
TECHNICAL COMPLEXITY	Difficult or impossible to model nonlinear chemistry and dispersion at long distances accurately.	Nonlinear chemistry of regional sources can be modeled, but plume overlap in mesoscale region is still a problem.	Nonlinear chemistry and regional plume dispersion can be treated accurately.
NEAR-SOURCE RESOLUTION (PSD)	Accurate, depending on plume segment resolution.	Accurate, depending on plume segment resolution.	Limited to size of grid cell.
COMPUTATION COST			
Single Source	Approx. \$100 per source-year	Approx. \$100 per source-year plus approx. \$5,000 for regional background	Approx. \$5,000 per source-year plus approx. \$5,000 for regional background
Multiple Sources (20 in mesoscale, 80 in large region)	Approx. \$10,000	Approx. \$2,000 plus approx. \$5,000 for regional background	Approx. \$5,000 plus approx. \$5,000 for regional background
Source Attribution (evaluating relative source contributions)	Small cost	Larger cost	Probably economically infeasible
SIMILARITY TO OTHER MODELS			
UNAMAP	Most similar	Most similar	Least similar
RADM	Least similar	Least similar	Most similar

Alternative 1: Fully Lagrangian Approach

This approach is probably the least costly for all potential applications, including analyses of single sources, cumulative impacts (e.g., 20 sources in a mesoscale area and 80 sources in a larger region), and source attribution (i.e., determining relative source and source category contributions). The approach is particularly appropriate for analyses where it is important to keep track of the specific contributions of individual sources. Calculating the relative contributions of several sources to deposition may be an important use of the Rocky Mountain Deposition Model. Eulerian approaches can be used for this purpose, but any attempt at a detailed analysis of source contributions using an Eulerian model would be prohibitively expensive.

However, there are two technical problems with a Lagrangian approach that must be dealt with if it is to yield accurate predictions. First, the chemistry and deposition of plume parcels is calculated independently of other air parcels; this creates problems when plume parcels overlap and chemical and deposition mechanisms are nonlinear (which they are for aqueous-phase reactions and wet deposition). Second, each plume is divided into discrete puffs or segments, each of which is transported with winds appropriate for the centroid of that segment; this method does not account for plume dispersion caused by wind shear and divergence over the width of the segment, as is prevalent in complex terrain.

There may be ways to account for the uncertainties caused by these problems with the Lagrangian approach. On the other hand, because the approach is similar to existing UNAMAP models used for PSD permitting work and has a low computational cost, it may be most acceptable to the end user. Its advantage for analyzing the relative contributions of multiple sources is a strong plus.

Alternative 2: Lagrangian/Eulerian Combination

Most of the problems associated with an exclusively Lagrangian approach might be solved with a "hybrid" approach, using a Lagrangian model for the mesoscale area and an Eulerian model in the larger region. This approach is essentially the same as the first with the addition of having an Eulerian model calculate inputs for the Lagrangian model. The Eulerian model, with a complete chemical mechanism or a parameterized version, would be used to calculate boundary conditions for the mesoscale region and the background reactivity (i.e., concentrations of O_3 , H_2O_2 , and OH , important in sulfate and nitrate formation) of the smaller region. Since the Eulerian approach would properly account for the nonlinear chemistry

of the emissions sources in the region, the uncertainties of the Lagrangian approach would be reduced. For example, if one were modeling only one source or group of sources in the smaller region, problems associated with plume overlap and long-distance dispersion would be less severe.

The regional (Eulerian) model would not necessarily have to be documented and delivered to the user; it could be applied every two or three years by a consultant who would supply the model output to the end user for input to the mesoscale Lagrangian model. Thus, costs for single-source evaluations would be kept relatively low while solving the problems associated with the fully Lagrangian approach. However, two models (Lagrangian and Eulerian) rather than one would need to be developed. Model evaluation of the Lagrangian component would be difficult. The regional Eulerian model could be evaluated by comparison with field measurements, then calculations of the mesoscale version of the Eulerian model could be compared with those of the Lagrangian mesoscale model. However, due to the lack of source-receptor data, no direct comparison of Lagrangian mesoscale model calculations with measurements could be made.

Alternative 3: Nested Eulerian Approach

The two major technical problems associated with the first two alternatives--dealing with nonlinear chemistry and large plume segments--would be eliminated with the third alternative. This approach uses the same grid model for both scales. The regional scale would be modeled with large grid squares, perhaps 100 km across, while the mesoscale region would be modeled with small grid squares, perhaps 2-5 km across, to provide higher resolution.

However, the technical advantages would cost considerably more. For an analysis of a single source, which is typical of PSD analyses, the nested model approach might cost \$5,000 in computer resources, whereas a Lagrangian model could be exercised for \$100. If the user could afford costs of approximately \$5,000 per source-year (perhaps by passing on the costs to the applicant), this approach may be attractive for technical reasons. For large modeling analyses, involving perhaps 100 sources in a region, the Eulerian approach may be no more expensive than the Lagrangian approach. However, for source attribution studies (i.e., identifying the relative contributions of different sources in different states to deposition in a given sensitive area), the Eulerian approach is likely to be prohibitively expensive.

Although the model would most likely be acceptable to the scientific community, the model formulation would be quite different from other models

with which the user is most familiar. However, the Eulerian model, like the Lagrangian model, could be applied as a "black box," without the need for detailed understanding of the inner workings of the "black box." The Eulerian approach would be most similar to NCAR's RADM and the engineering version of RADM.

6 CONCLUSIONS

An acid deposition model for the Rocky Mountain region is to be designed for use by regulatory agencies in the western states. After reviewing and selecting mesoscale meteorological and acid deposition models appropriate to application in the Rocky Mountain region, three alternative modeling approaches were identified. The modeling approach taken will depend upon the recommendations of the regulatory agencies. The resulting modeling system should be operational by the end of summer 1987.

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